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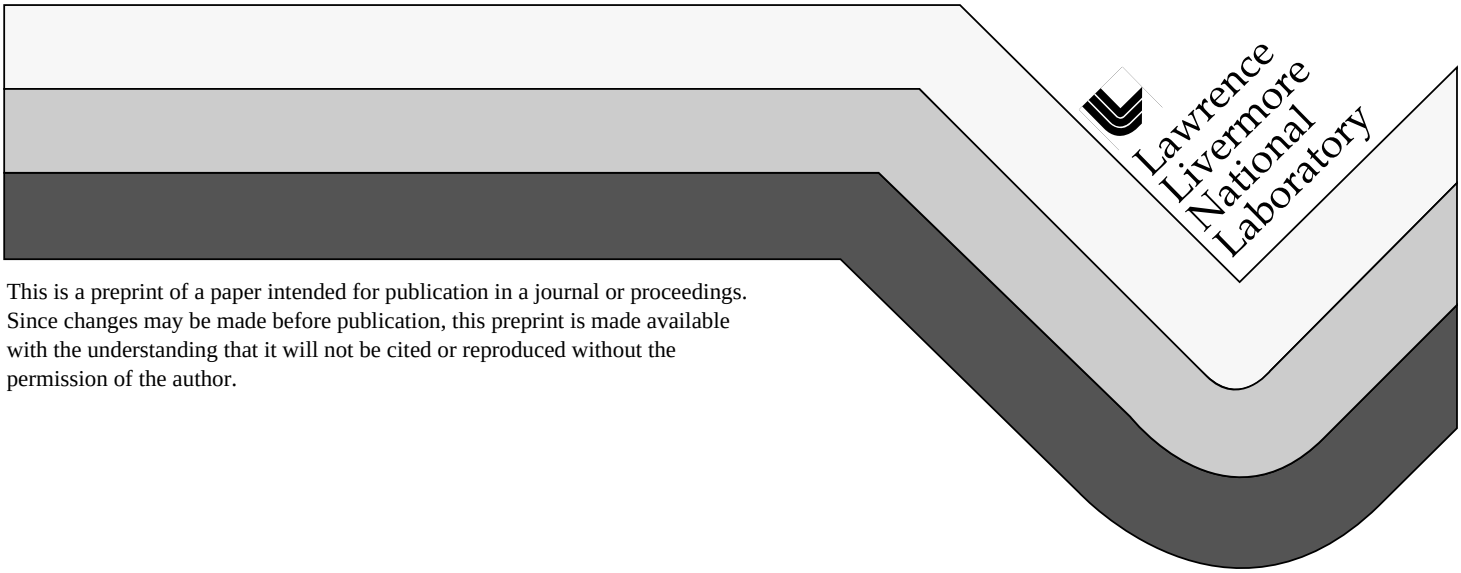

# LINKING *ab initio* ENERGETICS TO EXPERIMENT: KINETIC MONTE CARLO SIMULATION OF TRANSIENT ENHANCED DIFFUSION OF B IN Si

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## ABSTRACT

We have developed a kinetic Monte Carlo (kMC) simulator that links atomic migration and binding energies determined primarily from first principles calculations to macroscopic phenomena and laboratory time scales. Input for the kMC simulation is obtained from a combination of *ab initio* planewave pseudopotential calculations, molecular dynamics simulations, and experimental data. The simulator is validated against an extensive series of experimental studies of the diffusion of B spikes in self-implanted Si. The implant energy, dose, and dose rate, as well as the detailed thermal history of the sample, are included. Good agreement is obtained with the experimental data for temperatures between 750 and 950 C and times from 15 to 255 s. At 1050o C we predict too little diffusion after 105 s compared to experiment: apparently, some mechanism which is not adequately represented by our model becomes important at this temperature. Below 1050o C, the kMC simulation produces a complete description over macroscopic time scales of the atomic level diffusion and defect reaction phenomena that operate during the anneals. This simulator provides a practical method for predicting technologically interesting phenomena, such as transient enhanced diffusion of B, over a wide range of conditions, using energetics determined from first-principles approaches.

## INTRODUCTION

The continuing miniaturization of integrated circuits places ever more strict constraints on the size of the source and drain regions of field effect transistors (FETs). These highly doped regions of a silicon wafer are usually created by ion implantation of the dopant. After ion implantation, wafers must be annealed to remove damage caused by the implant and to electrically activate the dopant. During this annealing, the excess population of defects in the silicon can cause the dopant to diffuse orders of magnitude faster than it does under equilibrium conditions. As gate lengths decrease far below 1 m, such transient enhanced diffusion (TED) can become a very serious problem, as the dopant moves both deeper into the substrate and laterally, changing the gate length. The energy and dose of the implant, the highest temperature achieved, and the detailed thermal history (e.g., temperature ramp rates) all influence the final dopant profile. Thus it is important to know what combination of these variables leads to the most favorable ultimate dopant profile.

Experiments to separate the influence of each variable for each new generation of technology are expensive and time-consuming. The ultimate goal of our work is to develop a truly predictive model of dopant TED. Thus, given the implant species, energy, dose, and dose rate, the detailed thermal history, and the impurity concentration, the model would produce the correct three dimensional final dopant profile, as well as the degree of activation of the dopant and the damage remaining in the silicon. Previous approaches to this problem have typically relied on a set of parameters that had to be fitted in order to reproduce particular experimental observations. In order to be more fully predictive, we base our model on an extensive set of fundamental physical parameters for diffusion and clustering. If we accurately capture the essential physical processes, the model should be predictive over a very wide range of conditions.

The development of such a model is complicated by the huge range of time and length scales involved. Phenomena such as the diffusion of dopants require long time scales, on the order of minutes to hours. However, during ion implantation a dopant atom deposits its energy

into the lattice in just a few picoseconds. Device dimensions are on the order of a micron, yet the fundamental diffusive jumps are a fraction of a nanometer. Therefore, it is necessary to use an atomic-scale model with laboratory-scale predictive capabilities.

Our approach has been to develop a kinetic Monte Carlo simulator, which takes as input energies and prefactors from *ab initio* planewave pseudopotential calculations (for the dopant, impurity, and defect energetics), molecular dynamics simulations (for Si interstitial and vacancy diffusion and cluster binding energies), and fundamental experiments (for diffusion prefactors and very large Si interstitial cluster binding energies). It produces a three dimensional, atomic-scale description of dopant, defect, and impurity diffusion and clustering, on laboratory time and length scales. In this study, we apply the simulator to TED of B in Si, an important system in the production of FETs. The model is validated against an extensive series of experimental studies of the diffusion of B spikes in self-implanted Si. Details of the model and experiments are given in the next section. The results are discussed, and the areas in which the model currently falls short are presented along with those in which it succeeds remarkably well. Finally we conclude and indicate future directions for this work.

## METHOD

### Simulation

The basic input data necessary for the simulation of dopant diffusion are migration energies and binding energies of vacancies (Vs), self-interstitials (Is) and dopants. These values can be obtained from different sources, both theoretical and, in some cases, experimental. Recent computer simulations have provided a better understanding of defect production, diffusion, and clustering in Si. V and I formation and migration energies have been obtained using *ab initio* simulations (1-3), tight binding molecular dynamics (MD) (4) and empirical MD (5). Binding energies for I clusters and for V clusters have been obtained using Stillinger-Weber MD and tight binding MD models (4, 5). The interactions between dopants, impurities (e.g., C), and defects have also been studied using *ab initio* calculations. These can provide accurate information about the migration path of B (1, 3), about its binding energy in clusters with Is, and about the trapping of Is by C (6, 7).

B diffuses via an interstitial kick-out mechanism. After an I binds with a substitutional B atom to form a BI cluster, the Si atom may replace the B atom on the substitutional site, "kicking out" a mobile B interstitial, Bi. Our clustering model assumes that I and Bi spontaneously join any clusters they encounter, without an energy barrier. Clusters with two B atoms and three Si atoms (B2I3) and with three B atoms and two Si atoms (B3I2) are unstable with respect to emitting a Si interstitial to form B2I2 and B3I, respectively. The B3I cluster is particularly stable, and in this simulation essentially all of the inactive B fraction is found in B3I clusters. Clusters containing more than four B atoms were not considered, as they do not appear to be important for the B concentrations we are studying here.

Diffusion prefactors for Is and Vs were obtained from MD simulations. The diffusion prefactor for Bi was found by running a kMC simulation in a box with one I and one (initially substitutional) B, and adjusting the prefactor until the B diffusivity matched the experimental value. The prefactor for I diffusion was used for clusters that breakup by emitting an I; likewise that for Bi was used when clusters emit a Bi. These are reasonable estimates. However, these prefactors for cluster dissolution are not independently calculated or experimentally determined, and it is not unreasonable to treat them to a limited extent as adjustable parameters.

The dopant and damage profiles after implantation can be accurately modeled by binary collision codes, such as UT-Marlowe (8). UT-Marlowe allows simulation of different implanted species, energies, angles and doses in Si. In the binary collision approximation, two atoms interact according to a simple repulsive interatomic potential. The implanted ion undergoes a series of binary collisions with the lattice atoms. The recoiling lattice atoms collide with other lattice atoms, and so on. Thus the simulation also provides information about the cascade of defects produced by each implanted ion; that is, the location of all the Vs and Is produced during irradiation. The defect distribution obtained from this model is valid for irradiation with light ions, when the damage is primarily in the form of V-I pairs (Frenkel pairs) and no direct amorphization is produced by the implanted ions. Only the defects produced by ion implantation are considered

in our kMC simulation. At the temperatures studied here, the concentration of thermally excited defects in Si is expected to be negligible compared to that produced by cluster dissolution after the implant.

Our computationally efficient kMC model is based on that of Heinisch (9). As a function of time, it tracks the locations of defects, dopants, impurities, and extended defects (clusters). The various species are all treated as point particles with basic attributes that include size and diffusivity. During the simulation the particles participate in certain events. The possible events are: the dissociation of a particle from a cluster, with rate determined by the binding energy of the cluster; the diffusive jump of a particle, where the rate depends on the migration energy; and the introduction of a new cascade, that is, a new implanted ion and all its associated Vs and Is. The rate of cascade introduction is the dose rate of the simulated implantation. At each time step, we randomly choose among all possible events, ensuring that events occur at the proper rate by assigning each event a probability proportional to its rate. Following each chosen event, we perform all events that occur spontaneously as a result of that event. For example, an I that jumps within the capture radius of an I cluster then spontaneously joins the cluster. The simulation time is incremented by the inverse of the sum of the rates for all possible events in the simulation box. (Thus the model takes longer time steps when fewer events can occur.) The process then repeats. Because kMC focuses only on important particles and events, time scales of hours can be reached with these simulations. Clearly, great care must be taken to completely enumerate the relevant particles and events.

**Experiment**

The simulator was tested against a series of experimental studies of B TED. The test structures differed from FET structures in two important ways. First, rather than doping the sample by implanting B ions, the test structures were grown by chemical vapor deposition (CVD). They consisted of several B concentration spikes of amplitude 1x1019 cm-3 created during the deposition of a 1 μm thick epitaxial Si layer. Implant damage was created by subsequently bombarding the structure with 5x1013 Si ions/cm2 at 50 keV, up to a dose of 5x1013 ions/cm2. In such a structure the B layers can serve as markers for I diffusion. The second difference from FET structures is that the test samples are uniform in the plane of the wafer. Thus only depth information is relevant. A rapid thermal anneal (RTA) was performed at temperatures between 750 and 1050 C for times between 15 and 255 s. Temperature ramp rates for the RTAs were 150 C/s for the 750 C anneals and 100 C/s for the others. Additional furnace anneals were done at 750 C for times up to 10 hours. The total B concentration as a function of depth was determined by secondary ion mass spectrometry (SIMS).

## RESULTS

We assume a uniform background C concentration of $1 \times 1016$ cm-3, which is reasonable for CVD Si. Additionally, we assume that the front surface of the sample is a perfect sink for V, I, and Bi. As discussed above, it is reasonable (within limits) to treat the prefactors for cluster dissolution as fitting parameters. We adjusted the prefactor for the dissolution of the BI pair down by a factor of one-third from the prefactor for I diffusion, and that for the B3I dissolution up by a factor of two from the prefactor for Bi diffusion, in order to improve the match to the experimental data. The same prefactors were used in all the simulations presented here.

Results of the simulations are shown in Fig. 1. The as-grown B profile, taken as input to the simulations, is shown by the dashed line. The experimentally determined total B profile after annealing is shown as the solid line in each plot. The simulated total B profile is marked by filled circles, and the concentration of B3I clusters is marked by xs. Fig. 1a) and b) show good agreement between the simulations and experiments for both 15 and 255 s at 750o C. Note that the concentration of B3I clusters is the same at 15 s and at 255 s. In fact, all B3I clusters in the simulation form during the initial temperature ramp. Fig. 1c) shows excellent agreement between experiment and simulations after 195 s at 850o C. The predicted profile of B3I clusters is the same as in the 750o C simulations. Reasonable agreement is also obtained for 150 s at 950o C (not shown), although the simulation predicts too little diffusion in the deepest B peak. Some of the

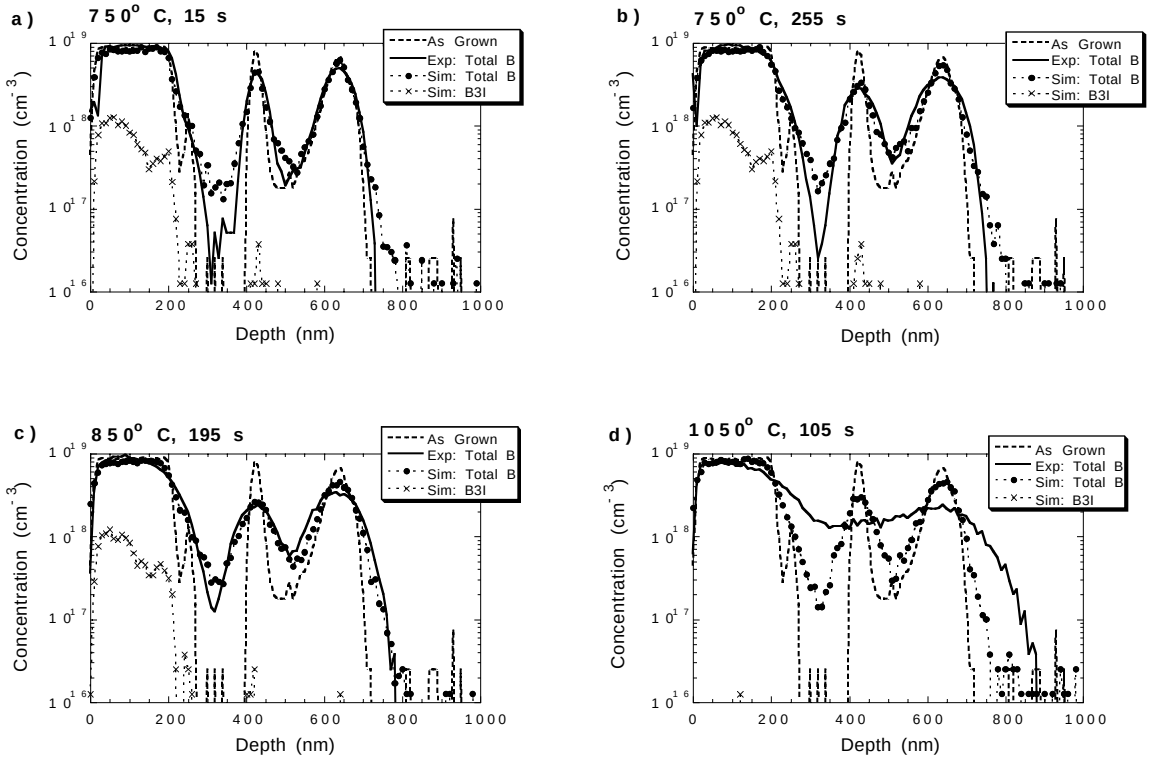


Fig. 1. Comparison of simulations and experimental results. As grown total B profiles shown by dashed line. Experimental results for total B concentration after RTAs shown by solid lines. Simulation results for total B shown by filled circles, for B3I clusters shown by xs. a) 750o C anneal, 15 s. b) 750o C anneal, 255 s. c) 850o C anneal, 195 s. d) 1050o C anneal, 105 s.

B3I clusters that form during the initial temperature ramp have dissolved after 150 s at 950o C. Unfortunately, the 1050o C simulation grossly underestimates the experimental diffusion, as shown in Fig. 1d). Experimentally, the deeper two B peaks have completely merged and become a shoulder on the first peak, whereas the model still predicts three distinct peaks. Further, all B and I clusters have dissolved and all defects have been eliminated from the simulation box by 60 s simulation time. It appears that some additional mechanism becomes important at this temperature which is not accounted for in the model.

## CONCLUSIONS AND FUTURE DIRECTIONS

We are approaching a predictive model for TED of B in Si. Good agreement has been obtained with RTA data for temperatures between 750 and 950 C and times between 15 and 255s. The only parameters adjusted to improve this fit are the prefactors for the breakup of the BI and the B3I clusters.

The B3I clusters are predicted to form during the initial ramp to high temperature, and not to dissolve at temperatures up to 850 C. The fraction of B which is electrically active (not clustered) is influenced by the temperature ramp rate, even though in these samples all the B is initially electrically active.

Further work is required to improve the behavior of the model at 1050 C. It is possible that at this temperature the equilibrium concentration of defects -- although there would be an average of less than one thermally excited defect in a volume the size of the simulation box at any time --

may be so mobile as to have a significant effect. We are in the process of investigating the influence of the low concentration of thermally excited defects. Dislocation loops can be formed after ion implantation, although generally not at the doses studied here. However, dislocation loops change the kinetics of interstitial clustering and dissolution, extending the time over which interstitials are available. Thus we plan to add dislocation loop formation to our kMC code in the future. Finally, the concentration of Si vacancies and interstitials predicted by UT-Marlowe has not been as extensively tested as its predictions of dopant profiles, and may be causing problems in our simulation. We plan to check the defect concentrations produced by UT-Marlowe against MD simulations of Si implants at the energies of interest.

Work is currently underway to improve our B clustering model using improved *ab initio* total energy calculations. Additionally, we are incorporating prefactors for Si V and I diffusivities determined from experimental results. (10) In the future, as we simulate lower energy implants and higher local dopant concentrations, we will need to incorporated the effects of shifting the Fermi level within the sample. This will have two effects. First, the diffusion rate and direction of charged species will be influenced by electric field gradients caused by a spatially varying Fermi level. Second, the relative populations of differently-charged species will be changed.

In future experimental work, we plan to validate the B clustering model using a combination of spreading resistance profiling and Hall measurements. Finally, additional time evolution information at higher temperatures will provide a check on our activation energies.

Although many refinements remain to be made, the results of this study are highly encouraging. We are approaching a model with enough of the necessary physics in it that a good approximation of reality is produced, over a range of conditions and with a minimum of fitting. Additional work should enable us to accurately link microscopic time and length scales to a fuller range of the conditions of interest in the laboratory or fabrication facility.

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